

# Bound states in a nonlinear Kronig Penney model

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## Abstract

We study the bound states of a Kronig Penney potential for a nonlinear one-dimensional Schrodinger equation. This potential consists of a large, but not necessarily infinite, number of equidistant  $\delta$ -function wells. We show that the ground state can be highly degenerate. Under certain conditions furthermore, even the bound state that would be normally the highest can have almost the same energy as the ground state. This holds for other simple periodic potentials as well.

# 1 Introduction

In this paper we shall study an unusual generalization of the one-dimensional Kronig Penney model. We shall examine in particular the spectrum of the bound states for a Kronig Penney potential  $V(z)$ , having added though a nonlinear term to the Schrodinger equation. Our arguments will be valid in the case of other simple periodic potentials as well.

Such nonlinear equations with periodic potentials arise in the Ginzburg-Landau treatment of various phenomena in condensed matter physics. In layered superconductors for example, such as the high temperature ones, a periodic potential such as the Kronig Penney potential can describe the periodically modulated superconductivity of the samples [1]. Spatially varying parameters in the nonlinear Schrodinger equation were also used to describe the periodic variation of the impurity concentration in superconductors [2], high  $T_c$  Josephson field effect transistors [3], as well as grain boundaries in superconducting bicrystals [4], while nonlinear Kronig Penney models were used for studying twinning-plane superconductivity [5]. The nonlinear Schrodinger equation must be used in order to describe all these various phenomena, including the relevant phase transitions. The nonlinear Schrodinger equation has been studied repeatedly, but mostly in regard to its solitons [6], and usually for nonperiodic potentials. In this work the emphasis is placed on studying the bound states, rather than solitons.

We shall study the excited states for the equation

$$-\frac{\hbar^2}{2M}\frac{\partial^2\Psi}{\partial z^2} + V(z)\Psi + \beta|\Psi|^2\Psi = 0. \quad (1)$$

The nonlinear term forbids the arbitrary normalization of  $\Psi$ .

The potential we have in mind is a Kronig-Penney potential, but it could be in general any simple oscillatory potential. In this work we choose

$$V(z) = V_0\left[1 - \alpha\sum_n\delta\left(\frac{z}{d} - n - \frac{1}{2}\right)\right], \quad (2)$$

with  $\alpha$  and  $V_0$  positive. The crucial parameter in this potential is the periodicity

length  $d$ . The number of wells is large, but not necessarily infinite.

Equation (1.1) minimizes the energy functional

$$\int dz \left[ V(z)|\Psi|^2 + \beta|\Psi|^4/2 + \frac{\hbar^2}{2M} \left| \frac{\partial \Psi}{\partial z} \right|^2 \right]. \quad (3)$$

For  $M \rightarrow \infty$  we would have  $|\Psi|^2 = -V(z)/\beta$ , in which case  $|\Psi|^2$  would follow the periodicity of  $V(z)$ . If the nonlinear term is omitted, the usual Kronig Penney model is recovered. In that limit  $-V_0$  is the energy, and  $\alpha V_0$  is the strength of each attractive delta function.

We can write the energy functional in dimensionless form, by measuring  $z$  in units of  $d$ , the distance between successive spikes of the potential,  $\Psi$  in units of  $\sqrt{V_0/\beta}$ , and the energy in units of  $dV_0^2/\beta$ , where  $V_0$  is the positive constant that appears in Eq. (1.2), and has the dimensions of  $V(z)$ . This constant is taken out of  $V(z)$ , so as to render it dimensionless. In other words,  $V(z)/V_0 = u(z)$ , where  $u(z)$  is dimensionless. If we define then the dimensionless parameter  $\nu = \hbar^2/2MV_0d^2$ , the energy functional takes the dimensionless form

$$\int dz \left[ u(z)|\Psi|^2 + |\Psi|^4/2 + \nu \left| \frac{\partial \Psi}{\partial z} \right|^2 \right]. \quad (4)$$

Note that when the quartic term is omitted, we recover the usual linear Kronig Penney model, with energy  $E = -\hbar^2/2M\nu d^2$ . In this case the energy values can be found only after imposing periodic boundary conditions on  $|\Psi|^2$ . There are then only certain allowed values of  $\nu$ , for a given value of  $\alpha$ . The size of the wavefunction is determined by the normalization, and when we minimize the energy functional under this constraint, we find the energy eigenvalues, i.e. the minima of the energy functional.

In the nonlinear case on the other hand, the size of  $\Psi$  is determined by the nonlinear terms, through the unconstrained minimization of the functional of Eq. (1.4). These nonlinear terms determine fully the behaviour of  $\Psi$ , without any need for boundary conditions. In fact, a periodic  $u(z)$  will give a periodic  $|\Psi|^2$ . Furthermore, the parameters  $\alpha$  and  $\nu$  are now independent, and for any pair of

values of  $\alpha$  and  $\nu$  we can find a solution  $\Psi$ , as long as  $\alpha$  is sufficiently large. We shall see later what is precisely the lower bound on  $\alpha$ . The energy of each state will be simply the value of the energy functional (1.4) at its minimum.

We see from Eq. (1.4) that for  $\nu \rightarrow 0$ , when the potential is very strong, or very weakly periodic, we get  $|\Psi|^2 \rightarrow -u(z)$ . Thus  $\Psi$  follows very closely the periodicity of the structure, since it can change very abruptly. In this limit though the sign of  $\Psi$  is arbitrary. So if the spikes of the potential are very far apart ( $d$  is long), the sign of  $\Psi$  could be positive or negative at each spike (see Fig. 1a).

Let us now switch on slowly the parameter  $\nu$ , bringing the teeth of the potential comb closer together. Then the wavefunction between neighboring spikes could have two forms. If the wavefunction on two successive spikes A and B is positive, say, then the wavefunction in the intervening region will be reduced, and it will go through a positive minimum value, remaining always positive though (Fig. 1b). If however the wavefunction changes sign in going from spike B to spike C, then it must pass through a point halfway between the spikes where it is exactly zero (see Fig. 1b). Since the wavefunction  $\Psi(z)$  minimizes the functional of Eq. (1.4), the energy equals  $-\int dz |\Psi|^4/2$ , as can be deduced by combining the dimensionless forms of Equations (1.1) and (1.3). Consequently the wavefunction has less energy if it does not go through zero, maintaining always the same sign. Indeed, in that case the minimum of  $|\Psi|^4/2$  is not zero, and hence the area under  $|\Psi|^4/2$  is greater.

It seems therefore more favorable for the wavefunction to have the same sign on all spikes of the potential. We say that the ground state is a *uniformly positive* state then. If the spikes of the potential are too far from each other however, then the minimum value of the wavefunction between them is practically zero, and in that case the *uniformly positive* state (where  $\Psi$  has the same sign at all spikes) becomes degenerate in energy with states that may have  $\Psi$  take on negative values at some spikes, and positive values at others.

We can, for example, have a state that is infinitesimally higher in energy

compared to the uniformly positive ground state, and hence practically equally preferable, even for spikes not too far apart. This state, with  $\Psi(0) = 0$ ,  $\Psi(z) > 0$  when  $z > 0$ , and  $\Psi(z) < 0$  when  $z < 0$ , connects regions of different signs of the wavefunction (see Fig. 2). Then in the intermediate region  $\Psi$  has to go through zero, and we get a region that reminds us of a domain wall. For a potential with *infinitely* many spikes, the energetically costly root of  $\Psi$  occurs only once, and hence the energy of this state is equal to the energy of the uniformly positive ground state.

There can be bound states of Equation (1.1) therefore that are degenerate to the ground state, not being everywhere positive. It is the purpose of this paper to study such bound states, first through a general variational model (Section 2), and then through an exact study of the Kronig-Penney potential (Section 3), as well as through a numerical study of a periodic potential with gaussian wells (Section 4). We summarize our conclusions in Section 5.

## 2 Variational Study

In this section we shall examine the possibility of having  $\Psi$  change sign in going from one spike of the potential to the next, as well as the possibility of having  $\Psi$  keep the same sign on neighboring spikes. In the first case  $\Psi$  is odd with respect to the midpoint between the two spikes, while in the second case it is even. An arbitrary state of the system will then be a combination of even and odd pieces. In other words,  $\Psi$  will be even between certain neighboring spikes of the potential, and odd between others. Thus  $\Psi$  will maintain its sign between some spikes, and it will change sign between others. For example, in Fig. 1b  $\Psi$  is odd in one interval, and even in the other two, while in Fig. 2 it is even everywhere, except for the interval at the center.

We have assumed that the spikes of the potential are at  $z = n + \frac{1}{2}$ , where  $n$  is any integer. Let us examine then the two neighboring quantum wells at the ends of the interval  $[n - \frac{1}{2}, n + \frac{1}{2}]$ . We adopt the following odd and even

trial wavefunctions, with respect to the midpoint ( $z = n$ ), defined on the interval  $[n - \frac{1}{2}, n + \frac{1}{2}]$ :

$$\Psi_{on}(z) = \pm\psi \frac{\sinh[\gamma(z - n)]}{\sinh(\gamma/2)}, \quad (5)$$

$$\Psi_{en}(z) = \pm\psi \left[ \frac{\cosh[\gamma(z - n)]}{\cosh(\gamma/2)} - \text{sech}^2(\gamma/2) \right] \coth^2(\gamma/2), \quad (6)$$

where  $\psi$  and  $\gamma$  are variational parameters. We note that  $\Psi_{on}(n) = 0$ ,  $\Psi_{on}(n + \frac{1}{2}) = -\Psi_{on}(n - \frac{1}{2}) = \pm\psi$ , and  $\Psi'_{on}(n + \frac{1}{2}) = \Psi'_{on}(n - \frac{1}{2}) = \pm\psi\gamma \coth(\gamma/2)$ . Similarly  $\Psi_{en}(n) = \pm\psi[\cosh(\gamma/2) - 1]/\sinh^2(\gamma/2)$ ,  $\Psi_{en}(n + \frac{1}{2}) = \Psi_{en}(n - \frac{1}{2}) = \pm\psi$ , and  $\Psi'_{en}(n + \frac{1}{2}) = -\Psi'_{en}(n - \frac{1}{2}) = \pm\psi\gamma \coth(\gamma/2)$ .

These wavefunctions are such that they can be joined together in any order to form a continuous wavefunction everywhere, consisting of even and odd pieces. We could have, for example,  $\Psi = \Psi_{on}$  in  $[n - \frac{1}{2}, n + \frac{1}{2}]$ ,  $\Psi = \Psi_{e,n+1}$  in  $[n + \frac{1}{2}, n + \frac{3}{2}]$ ,  $\Psi = -\Psi_{o,n+2}$  in  $[n + \frac{3}{2}, n + \frac{5}{2}]$ , etc. Furthermore, regardless of the order in which the even and odd pieces are connected, the slope of the wavefunction is symmetric around the spikes of the potential.

The state with the lowest energy would consist of a chain of even pieces, because, unlike the odd pieces which have a root at the midpoint, the even pieces are nowhere equal to zero. Thus the odd pieces have a higher  $-\int dz |\Psi|^4/2$ , which is the exact energy if  $\Psi$  is an exact solution of the equations that minimize the energy functional.

The next lowest energy would correspond to the state with only one odd piece. This is the state of Fig. 2. It is presumed here though that the change from the chain of negative pieces to the chain of positive pieces occurs within just one spacing. The circumstances under which this will happen will be explored later.

The state mentioned above is followed by the state with two odd pieces, and so on, up to the highest state, which has only odd pieces. In fact, if  $F_e$  and  $F_o$  is the energy in  $[n - \frac{1}{2}, n + \frac{1}{2}]$  for the even and odd trial wavefunctions respectively, then the energy of a state with  $m$  even pieces and  $n$  odd pieces is  $mF_e + nF_o$ . Thus the total energy per interval is  $(mF_e + nF_o)/(m+n)$ . In particular, the energy per

interval is  $F_e$  for the uniform chain of even pieces, i.e. the ground state, and  $(mF_e + F_o)/(m+1)$  for the state with only one odd piece, i.e. the state of Fig. 2. For an *infinite* number of spikes ( $m \rightarrow \infty$ ), the two states are *degenerate*, as expected. Of course, the same holds for a state with infinitely many even pieces, but only two odd pieces. If the number of odd pieces becomes substantial though, then the energy of the state will be definitely higher than that of the ground state.

For a large but finite number of spikes we still expect all these various states to be degenerate, as long as the minimum value of the even pieces is practically zero, because in that case  $|\Psi|^4$  is essentially the same for both even and odd pieces. We shall verify this by explicit calculation, using our variational wavefunctions.

We note that  $\Psi_{en}(n) \rightarrow 0$  when  $\gamma \rightarrow \infty$ . Therefore the degeneracy mentioned above requires that  $\gamma$  be very large. We shall neglect therefore terms like  $\text{sech}(\gamma/2)$ . In this limit,

$$F_e \approx \nu\gamma|\psi|^2 + \frac{|\psi|^4}{4\gamma} + \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dz u(z)|\psi|^2 \frac{\cosh^2[\gamma(z-n)]}{\cosh^2(\gamma/2)} + O(e^{-\gamma}) \quad (7)$$

$$F_o \approx \nu\gamma|\psi|^2 + \frac{|\psi|^4}{4\gamma} + \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dz u(z)|\psi|^2 \frac{\sinh^2[\gamma(z-n)]}{\sinh^2(\gamma/2)} + O(e^{-\gamma}). \quad (8)$$

Hence, since  $\cosh^2(\gamma/2) \approx \sinh^2(\gamma/2) \approx e^\gamma/4$ ,

$$F_o - F_e \approx - \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dz 4e^{-\gamma} u(z) |\psi|^2. \quad (9)$$

And since  $\gamma$  is large, and terms of order  $O(e^{-\gamma})$  have been dropped in this calculation, Eq. (2.5) implies that  $F_o \approx F_e$ . In other words, if  $\Psi_{en}(n) \approx 0$ , then all the possible states are practically degenerate, even for a finite large number of spikes, because they consist of odd and even pieces only, pieces which were shown to have the same energy. Note that our results are very general so far. The only restriction is that the  $\gamma$  that minimizes Eq. (2.3) be large. Our conclusions are valid though for *any*  $u(z)$  that can lead to a large  $\gamma$ .

We illustrate the above general conclusions by restricting ourselves now to the

Kronig-Penney model:

$$u(z) = 1 - \sum_n \alpha \delta(z - n - \frac{1}{2}). \quad (10)$$

This choice of  $u(z)$ , where  $\alpha$  is a positive constant, implies that there is a periodic chain of deep quantum wells along the  $z$  axis.

For this choice of  $u(z)$  then, and in the limit of large  $\gamma$ , we get

$$F_o \approx F_e \approx |\psi|^2 \left[ \nu\gamma + \frac{1}{\gamma} - \alpha \right] + \frac{|\psi|^4}{4\gamma}. \quad (11)$$

Minimization with respect to  $|\psi|^2$  gives

$$|\psi|^2 = 2\gamma \left[ \alpha - \nu\gamma - \frac{1}{\gamma} \right] \quad (12)$$

and

$$F_o \approx F_e \approx -\gamma \left[ \alpha - \nu\gamma - \frac{1}{\gamma} \right]^2. \quad (13)$$

Minimization with respect to  $\gamma$  yields

$$\gamma = \frac{\alpha + \sqrt{\alpha^2 + 12\nu}}{6\nu}, \quad (14)$$

or equivalently  $3\nu\gamma - \alpha = 1/\gamma$ , in which case  $|\psi|^2 = 4\nu\gamma^2 - 4$ . Since  $\gamma \gg 1$ , we shall have

$$\gamma \approx \alpha/3\nu \gg 1. \quad (15)$$

Since  $|\psi|^2 \geq 0$ , we must also have  $\gamma \geq 1/\sqrt{\nu}$ , which implies

$$\alpha^2 \geq 4\nu. \quad (16)$$

Whenever therefore  $\nu$  and  $\alpha$  satisfy the *restrictions* of Eqs. (2.11) and (2.12), we expect all the possible states to be essentially degenerate. In particular, the *highest* excited state, the one consisting of odd pieces only, is *degenerate* with the *ground* state, which is a chain of even pieces. Note furthermore that the wavefunction is nonzero only if  $\nu \leq \alpha^2/4$ . When in fact  $\nu = \alpha^2/4$ , we have a transition to a zero wavefunction, even though  $\gamma$ , which takes then the value  $1/\sqrt{\nu}$ , may be quite large.

As a numerical illustration, we choose the case  $\nu = 0.01$ ,  $\alpha = 1$ . Then the ground state and the highest excited state (only even or only odd pieces



respectively) have an energy of  $-13.5207$  in this variational model, with  $\gamma = 34.305$  and  $\psi = 6.56$ . The exact energy can be found using the methods of section 3, and it is  $-14.933$  for both the ground state and the highest state, while  $\psi = 6.93$ . So both calculations indicate that all the states are degenerate, for this particular choice of  $\nu$  and  $\alpha$ .

The example where  $u(z)$  is given by Eq. (2.6) will be examined also in section 3, since it can be solved exactly. We can generalize for *any* simple oscillatory  $u(z)$  though, so long as  $\gamma$  is very large.

### 3 Exact Solutions

In this section we shall solve exactly the model of Eqs. (1.4) and (2.6), verifying thus the variational results of the previous section. We shall be interested in *those* values of the parameters  $\nu$  and  $\alpha$  that yield excited states *almost degenerate* with the ground state.

We should note that a large  $\nu$  would imply that the kinetic energy is dominant, making thus the wavefunction too stiff. In other words, the ground state wavefunction would come as closely as possible to a constant, a choice that minimizes the kinetic energy. In that case the minimum value of the ground state wavefunction would be far from zero.

On the other hand, if  $\nu$  were exactly zero, then the wavefunction would follow the variations of  $u(z)$  exactly. Hence we need a small value of  $\nu$  if we are going to have an excited state that is close in energy to the ground state, since the wavefunction of such a state varies dramatically between the spikes. Furthermore, if  $\nu$  is zero the wavefunction will have arbitrary signs at the wells, in which case the various excited states will all be degenerate with the ground state. For small  $\nu$ , this degeneracy will not be altered too drastically.

We shall be interested therefore in the exact solutions of this model, for small

$\nu$ . The energy functional is minimized when

$$\nu \frac{\partial^2 \Psi}{\partial z^2} = \left[ 1 - \sum_n \alpha \delta(z - n - \frac{1}{2}) \right] \Psi + |\Psi|^2 \Psi \quad (17)$$

The solution  $\Psi(z)$  will have periodic features similar to those of  $u(z)$ . Integrating Eq. (3.1) gives the boundary condition for  $\Psi(z)$

$$-\alpha \Psi(n + \frac{1}{2}) = \nu \left[ \frac{\partial \Psi}{\partial z}(n + \frac{1}{2})_+ - \frac{\partial \Psi}{\partial z}(n + \frac{1}{2})_- \right]. \quad (18)$$

Thus  $\Psi(z)$  has a kink at each spike of the potential, due to the  $\delta$ -functions.

Direct integration of Eq. (3.1) after multiplying it by  $\partial \Psi / \partial z$  gives the solution in each interval. The ground state has no node, hence  $\Psi$  will have a minimum at the middle of each interval, while it will be symmetric around each spike. Thus the *exact* ground state is found to be

$$\Psi(z) = \frac{q}{cn \left[ \sqrt{(1+q^2)/\nu} (z-n), (2+q^2)/(2+2q^2) \right]}, \quad (19)$$

for  $n - \frac{1}{2} \leq z \leq n + \frac{1}{2}$ , extended periodically everywhere else. Here  $cn$  is a Jacobi elliptic function, and  $q = \Psi(n)$  is the minimum value of  $\Psi(z)$ . The above expression is valid for *any* value of  $\nu$ , large or small, and we can easily verify that it satisfies Eq. (3.1).

The boundary conditions of Eq. (3.2) require then that

$$\alpha = 2\nu \sqrt{\frac{1+q^2}{\nu}} \frac{sn \left[ \sqrt{\frac{1+q^2}{4\nu}}, \frac{2+q^2}{2+2q^2} \right] dn \left[ \sqrt{\frac{1+q^2}{4\nu}}, \frac{2+q^2}{2+2q^2} \right]}{cn \left[ \sqrt{\frac{1+q^2}{4\nu}}, \frac{2+q^2}{2+2q^2} \right]}, \quad (20)$$

where the  $dn$  and  $sn$  are also Jacobi elliptic functions. This equation determines  $q$  as a function of  $\alpha$  and  $\nu$ . Note that there is always a ground state, since we can always find an appropriate  $q$  for a given choice of  $\nu$  and  $\alpha$ .

In the limit of a wavefunction localized around the spikes of the potential we expect  $q$  to be small. Then Eq. (3.3) reduces to

$$\Psi(z) \approx q \cosh[(z-n)/\sqrt{\nu}]. \quad (21)$$

This is precisely the solution of the linear Kronig Penney model, as expected, since for very small  $q$  the nonlinear terms become unimportant. If  $q = 0$ , Eq. (3.4) yields

$$\alpha = 2\sqrt{\nu} \tanh(1/2\sqrt{\nu}). \quad (22)$$

So a nonzero ground state will exist only if  $\alpha \geq 2\sqrt{\nu} \tanh(1/2\sqrt{\nu})$ . Note that for small  $\nu$  this becomes the restriction of Eq. (2.12), as it should. Furthermore, if  $\alpha$  is close to its lower limit, then the change of sign of  $\Psi$  for a first excited state will have to spread over a few more spikes of the potential, and it will not be restricted to just the region between two successive spikes. In this paper we shall not be concerned with this possibility, and we shall restrict our attention to values of  $\alpha$  far from the lower bound of Eq. (3.6). Then the change of sign for the excited states occurs within just one spacing.

Now the Jacobi elliptic function  $cn(x, m)$  is a periodic function, with roots at the odd multiples of the elliptic function  $K(m)$ , where  $K(m) = \int_0^{\pi/2} d\theta / \sqrt{1 - m \sin^2 \theta}$ . Indeed,  $cn(0, m) = 1$ ,  $cn(K(m), m) = 0$ ,  $cn(2K(m), m) = -1$ ,  $cn(3K(m), m) = 0$ ,  $cn(4K(m), m) = 1$ .

The ground state, as mentioned in the previous section, must consist of even pieces everywhere, of the form given by Eq. (3.3). It must therefore be positive everywhere, since it is continuous. So the  $\Psi$  of Eq. (3.3) must not be allowed to become negative. This means that the quantity  $\sqrt{(1 + q^2)/\nu} |z - n|$  must be smaller than  $K((2 + q^2)/(2 + 2q^2))$  within the interval  $[n - \frac{1}{2}, n + \frac{1}{2}]$ . Hence

$$\frac{1}{2} \sqrt{(1 + q^2)/\nu} \leq K\left(\frac{2 + q^2}{2 + 2q^2}\right). \quad (23)$$

This inequality holds for any values of  $\alpha$  and  $\nu$ . If  $\nu$  is small, then the right hand side of this inequality has to be large. This happens when the argument of  $K(m)$  is close to 1, in which case  $K(m) \approx \ln \sqrt{16/(1 - m)}$ . In this particular case, the argument is 1 if  $q$  is very small. Thus if  $\nu$  is small,  $q$  must be small.

Furthermore, when inequality (3.7) becomes an equality, the denominator in Eq. (3.3) tends to zero at  $z = n + \frac{1}{2}$ , and therefore the value of  $\Psi(z)$  at the spikes

becomes infinite. In other words, the value of  $\Psi$  at the spikes can be much larger than the value of  $\Psi$  at the midpoints.

Indeed  $\Psi(n - \frac{1}{2})/\Psi(n) = 1/cn[\sqrt{(1+q^2)/4\nu}, (2+q^2)/(2+2q^2)]$ . Hence, if  $q \rightarrow 0$ ,  $\Psi(1/2)/\Psi(1) \approx \cosh(1/\sqrt{4\nu})$ , which tends to infinity when  $\nu$  tends to zero. Thus the even pieces of  $\Psi$  become very deep if  $\nu$  is small, because in that case  $q \rightarrow 0$  and  $\Psi(n \pm \frac{1}{2})$  is very large.

We say in that case that the wells are weakly coupled. Note that in that case the  $|\Psi|^4$  of an even piece would not differ too much from the  $|\Psi|^4$  of an odd piece. In other words, we expect the various possible states to be very close in energy to the ground state, as mentioned already in section 2. Indeed the case  $\nu = 0$  would correspond to a complete decoupling of the values of the wavefunctions at the spikes of the potential, and hence to a complete degeneracy of all the various states.

Let us examine more thoroughly the singularities that may arise in the behavior of  $\Psi$ . We said that  $\Psi(z)$  becomes very large at the spikes of the potential when inequality (3.7) becomes almost an equality:

$$\sqrt{(1+q^2)/4\nu} \approx K(\frac{2+q^2}{2+2q^2}). \quad (24)$$

But if  $m$  is very close to 1, then  $K(m) \approx \ln \sqrt{16/(1-m)}$ . Hence this approximate equality reduces for small  $q$  to  $1/2\sqrt{\nu} \approx \ln(\sqrt{32/q^2})$ , whence

$$q \approx \sqrt{32} e^{-1/2\sqrt{\nu}}. \quad (25)$$

Hence, if  $\nu$  is small, and if the ground state wavefunction has deep cups, we must have  $q \approx \sqrt{32} \exp(-1/2\sqrt{\nu})$ . Note that even though  $q$  is small, the value of the wavefunction at the minima of the potential is large. Nonetheless, since  $q \rightarrow 0$ , the wavefunction is again given by Eq. (3.5), an equation that tells us that  $\Psi(z)$  falls to  $1/e$  of its value within a distance of  $\sqrt{\nu}$  from the spikes. In that sense we can say that the "thickness" of  $\Psi$  at each spike is  $2\sqrt{\nu}$ . But the peaks of  $\Psi$  would overlap when the thickness of each peak equals the distance between successive peaks. This happens when  $\nu = 1/4$ . When we speak therefore of weakly coupled

wells, we mean that  $\nu \ll 1/4$ . And it is only such wells that can lead to an essentially degenerate spectrum of states.

Let us then summarize our results for the ground state. There is always a ground state, with  $q = \Psi(n)$  being the minimum value of  $\Psi$  in the interval  $[n - \frac{1}{2}, n + \frac{1}{2}]$ . This is a symmetric series of even pieces, and it resembles a chain of symmetric cups (see Fig. 3). The absolute value of the slope of  $\Psi$  at the layers is  $\alpha\Psi(n + \frac{1}{2})/2\nu$ . This ground state will be degenerate with any other states if their  $|\Psi|^4$ 's are approximately the same. This can happen only if  $q$  is almost zero, as explained in section 2, because then the minimum of the  $|\Psi|^4$  of the even piece approaches the minimum of  $|\Psi|^4$  of the odd piece, i.e. zero. But  $q$  can be tiny, and  $\Psi$  still have a substantially nonzero value, only close to the roots of the Jacobi elliptic function  $cn$  (see Eq. (3.3)), i.e. for  $q \approx \sqrt{32}e^{-1/2\sqrt{\nu}}$ . Furthermore,  $q$  needs to be small in order to have the degeneracy. Hence  $\nu$  must be small. Indeed, the thickness  $2\sqrt{\nu}$  of each well implies that the wavefunctions around the spikes will not overlap substantially, provided  $\nu \ll 1/4$ . For small  $\nu$  then we get a ground state which resembles a chain of deep cups (see Fig. 3).

Let us now proceed to the first excited state (see Fig. 2). Here we assume again that  $\nu$  is small, and hence the even pieces will resemble deep cups. There will be only one odd piece, in the interval  $[-1/2, 1/2]$ , connecting a chain of negative even pieces with a chain of positive even pieces. The characteristics of the many even pieces will not be altered, because there is only one odd piece. On the contrary, the characteristics of the odd piece will be determined from those of the even pieces, through the boundary conditions.

Direct integration of Eq. (3.1) after multiplying it by  $\partial\Psi/\partial z$  will give the solution in the interval  $[-1/2, 1/2]$ , as long as we use the fact that  $\Psi(0) = 0$ , since there is one node there. For the first excited state there is only one node,

thus all the pieces outside the interval  $[-1/2, 1/2]$  will be even.

One can show thus that for  $-1/2 \leq z \leq 1/2$  we get the *exact* solution

$$\Psi(z) = \sqrt{1-\epsilon} \frac{sn[z\sqrt{(1+\epsilon)/2\nu}, 2\epsilon/(1+\epsilon)]}{cn[z\sqrt{(1+\epsilon)/2\nu}, 2\epsilon/(1+\epsilon)]}, \quad (26)$$

with  $\Psi'(0) = \sqrt{(1-\epsilon^2)/2\nu}$  and  $0 \leq \epsilon \leq 1$ . We can easily verify that this expression satisfies Eq. (3.1). The value of  $\Psi(z)$  at  $z = 1/2$ , as calculated from Eq. (3.10), must be equal to the one that can be calculated from Eq. (3.3). This relation determines the parameter  $\epsilon$ . If the even pieces are deep enough, i.e. if  $\nu$  is small enough, then the slope of  $\Psi(z)$  at  $(1/2)_-$  will turn out to be  $\alpha\Psi(\frac{1}{2})/2\nu$ .

Indeed, we saw that if for small  $\nu$  the value of  $\Psi$  at the spikes of the potential is very large, then  $q \approx \sqrt{32}e^{-1/2\sqrt{\nu}}$ . In general, the even and odd pieces correspond to the same energy if  $\Psi$  is very large at the spikes,  $q$  being quite small. But if  $\Psi(1/2)$  is very large, then Eq. (3.10) implies that  $cn[\sqrt{(1+\epsilon)/8\nu}, 2\epsilon/(1+\epsilon)] \approx 0$ , so as to make  $\Psi(z)$  almost diverge. Consequently

$$\sqrt{(1+\epsilon)/8\nu} \approx K[2\epsilon/(1+\epsilon)], \quad (27)$$

where  $K$  is the elliptic function  $K(m) = \int_0^{\pi/2} d\theta/\sqrt{1-m\sin^2\theta}$ . And since  $\nu$  is small, the value of  $K$  will have to be rather large, which means that  $2\epsilon/(1+\epsilon) \rightarrow 1$ , i.e.  $\epsilon \rightarrow 1$ . Indeed, remembering that  $K(m) \approx \ln\sqrt{16/(1-m)}$  when  $m \rightarrow 1$ , we can easily find that Eq. (3.11) is solved by the value

$$1-\epsilon \approx 32e^{-1/\sqrt{\nu}}. \quad (28)$$

So this value of  $\epsilon$  yields a very large  $\Psi(1/2)$ , for small  $\nu$ . In fact, we must have in general, for any  $\nu$ ,

$$\sqrt{(1+\epsilon)/8\nu} \leq K[2\epsilon/(1+\epsilon)], \quad (29)$$

otherwise the elliptic function  $cn$  would get a root in  $[0, 1/2]$  and  $\Psi(z)$  would have a vertical asymptote there.

We can now check the value of  $\Psi(1/2)$ . The second argument of the elliptic functions  $sn$ ,  $dn$  and  $cn$  is  $(2+q^2)/(2+2q^2)$  for the even pieces and  $2\epsilon/(1+\epsilon)$  for

the odd pieces, both of which will equal  $1 - 16e^{-1/\sqrt{\nu}}$  when Eqs. (3.9) and (3.12) hold, i.e. for very large values of  $\Psi(1/2)$ . Therefore for very small  $\nu$  this second argument is essentially 1, in which case the  $sn$  becomes  $\tanh$ , the  $cn$  becomes  $sech$ , and the  $dn$   $sech$ . Then Eq. (3.10) gives  $\Psi(z) \approx \sqrt{1-\epsilon} \sinh(z\sqrt{(1+\epsilon)/2\nu})$  in  $[-1/2, 1/2]$ , and  $\Psi(z) \approx q \cosh[(z-n)/\sqrt{\nu}]$  in  $[n-\frac{1}{2}, n+\frac{1}{2}]$ , where  $n \neq 0$ . Both expressions give then the same values for  $\Psi(1/2)$  and  $|\Psi'(1/2)|$ , as expected.

The procedure for finding the first excited state then consists of finding the value of  $\epsilon$  that would ensure continuity of  $\Psi(z)$  at  $z = 1/2$ . In that case the slope at  $z = (1/2)_-$  will turn out automatically to be the exact opposite of the slope at  $z = (1/2)_+$ . Finding the ground state, on the other hand, simply requires finding a  $q$  such that  $|\Psi'(n + \frac{1}{2})| = (\alpha/2\nu)\Psi(n + \frac{1}{2})$ . This relation is precisely Eq. (3.4).

Finally, we can find the highest excited state, the one consisting of odd pieces only, by extending periodically the odd solution of Eq. (3.10), and finding a value of  $\epsilon$  such that  $|\Psi'(n + \frac{1}{2})| = (\alpha/2\nu)\Psi(n + \frac{1}{2})$ . Since the minimum value  $q$  of the even piece for the solutions that interest us is  $\sqrt{32}e^{-1/2\sqrt{\nu}}$ , i.e. practically zero, the energy of the even piece and of the odd piece is essentially the same since they have the same  $-\int dz|\Psi|^4/2$ . And all the states are then degenerate.

It is interesting to note that  $\alpha = 2\nu\Psi'(\frac{1}{2})/\Psi(\frac{1}{2}) \rightarrow 4\nu + \frac{1}{3}$  if  $\nu \rightarrow \infty$ , for the  $\Psi(z)$  of Eq. (3.10). Hence the highest state does not exist when  $\nu \rightarrow \infty$ , unless  $\alpha = 4\nu + \frac{1}{3}$ . Similarly, quite a few other excited states do not exist for large values of  $\nu$ . The even ground state exists always though, if  $\alpha$  is above the lower bound of Eq. (3.6). We present numerical values of the parameters and energies of the ground state, of the first excited state and of the highest state in Tables 1, 2 and 3 for various choices of  $\nu$  and  $\alpha$ .

Note that for a given choice of  $\nu$ , large or small, and a given value of  $\alpha$  greater than the lower bound of Eq. (3.6),  $q$  is given by Eq. (3.4). But it is only small  $\nu$ 's, and  $\alpha$ 's quite far from their lower bound, that will lead to a ground state with deep even pieces. In that case  $q$  is given by Eq. (3.9), and the ground state will be practically degenerate with the first few excited states.

## 4 A Potential With Gaussian Wells

We shall examine numerically the bound states that correspond to the choice

$$u(z) = 1 - g \sum_n \exp[-b(z - n - \frac{1}{2})^2], \quad (30)$$

shown in Fig. 4. We choose the parameters so that  $e^{b/4} > g > 1$ . Then  $u(z)$  is negative at its minima and positive at the midpoints between the minima. Therefore, if  $\nu$  were exactly zero, then there would be a nonzero wavefunction at the minima of  $u(z)$ , but there would be a region around the midpoints where  $\Psi$  would be exactly zero. When  $\nu$  is slightly positive, the stiffness of the wavefunction makes  $\Psi$  leak into the "forbidden" regions (tunnelling). If however  $b < 4 \ln g$ , then there is no tunnelling. We need a large enough  $b$  in order to get tunnelling.

If on the other hand  $b$  is extremely large, while  $g$  remains finite, the width of each well is reduced, its strength remaining unaltered. We expect therefore that for a given  $g$  we cannot increase  $b$  indefinitely, because we shall not be able to find a solution. The numerical calculations do indeed verify this.

Thus, if  $b$  is large enough, but not too large, and if  $g$  is large enough to allow a nonzero solution, we shall have a competition between the kinetic energy and the rest of the energy. The latter forces  $\Psi$  to follow the variations of  $u(z)$ . The kinetic energy, on the other hand, wants  $\Psi$  to be constant in space. Solutions such as the one of Fig. 2 will be relevant for small  $\nu$ , since large values of  $\nu$  tend to push  $\Psi$  towards a constant. Indeed, numerical calculations verify that for large  $\nu$  (e.g.  $\nu = 0.3$ ), the kinetic energy is strong enough to force  $\Psi_{max}$  to be close to  $\Psi_{min}$ , and  $\Psi_{min} \gg 0$ . The ground state is then a chain of shallow little cups away from zero.

Excited states that will be almost degenerate in energy with the ground state will appear at small values of  $\nu$ , when the minimum of the ground state wavefunction between the wells is very small, while  $\Psi_{max} \gg 0$ . Fig. 5 shows the ground state, the first excited state, and the highest excited state, for  $\nu = 0.01$ , with the corresponding energies per interval, for a sample of 20 gaussian wells.



Fig. 6 shows the same states, but for  $\nu = 0.05$ . We see again the characteristics mentioned earlier: full degeneracy if  $\nu$  is small enough, in which case the minimum of  $\Psi$  between wells is quite small compared to its value  $\Psi_{max}$  at the wells. The value of  $\Psi_{max}$  depends strongly on  $g$ .

Remember also that the energy difference between the ground state and the first excited state is strictly equal to zero for an infinite number of wells. This is due to the fact that the wavefunction of the first excited state is exactly equal or exactly opposite to the wavefunction of the ground state on almost all of the infinitely many wells. Indeed, in Figs. 7 and 8 we see the first excited state for a fairly large value of  $\nu$ , and a series of values for  $b$  and  $g$ . Here the stiffness of the wavefunction is quite large, so the change of the sign cannot take place within just one interval. This change now occurs over three or four wells. For small values of  $\nu$  though, when the wavefunction is quite malleable, the wavefunction changes sign within one interval.

## 5 Conclusions

We have studied the bound states of a nonlinear version of the Schrodinger equation for the Kronig Penney model, a version that is relevant to quite a few phenomena in condensed matter physics.

We have seen that there is a substantial range of parameters, not just for the Kronig Penney model but for other simple oscillatory choices of  $u(z)$  as well, for which the various states are essentially degenerate in energy. This degeneracy requires that  $\nu$  be small enough, so as to allow the wavefunction to have a small, but non-negligible, value at the midpoints between the wells. At the same time the value of the wavefunction at the wells can be quite substantial. Then there is very little cost in having  $\Psi$  change sign in going from one well to the next. In fact, the energy differences are really small when  $\Psi_{max} \gg \Psi_{min}$ . This means that the lower excited states, which connect regions of positive  $\Psi$  with regions of negative  $\Psi$ , become as favorable as the ground state. This degeneracy is exact in

the limit of infinitely many quantum wells for these lower excited states. Even the highest excited state though, which consists of odd pieces only, has an energy very close to the energy of the ground state for sufficiently small  $\nu$ .

We demonstrated this basic idea in Section 2 through a variational calculation valid for a generic oscillatory potential. The variational results were confirmed through the exact solution of the nonlinear Kronig Penney model, presented in Section 3, as well as through a numerical calculation for the case of another simple oscillatory potential, presented in Section 4. All these calculations show the exact (for infinitely many spikes) or approximate (for finitely many spikes) degeneracy of the ground state.

## References

- [1] T. Koyama, N. Takezawa, Y. Naruse, M. Tachiki, *Physica C* **194**, 20 (1992);  
T. Koyama, M. Tachiki, *Physica C* **193**, 163 (1992); M. Machida, H. Kaburaki, *Physical Review Letters* **74**, 1434 (1995); L. Balents, L. Radzihovsky, *Physical Review Letters* **76**, 3416 (1996).
- [2] S. Ami, K. Maki, *Progress of Theoretical Physics* **53**, 1 (1975).
- [3] J. Betouras, R. Joynt, Z. W. Dong, T. Venkatesan, P. Hadley, *Applied Physics Letters* **69**, 2432 (1996).
- [4] J. Betouras, R. Joynt, *Physica C* **250**, 256 (1995).
- [5] I. Khlyustikov, A. Buzdin, *Advances in Physics* **36**, 271 (1987); A. Abrikosov, A. Buzdin, M. Kubic, D. Kuptsov, *Soviet Physics JETP* **68**, 210 (1989).
- [6] K. Hizanidis, D. Frantzeskakis, C. Polymilis, *Journal of Physics* **A29**, 7687 (1996); D. Frantzeskakis, *Journal of Physics* **A29**, 3631 (1996); H. Frauenkron, P. Grassberger, *Journal of Physics* **A28**, 4987, (1995).

## Table Captions

**Table 1:** Parameters of the ground state for  $\delta$ -function wells, for various choices of  $\nu$  and  $\alpha$ .  $E_g$  is the energy per interval.

$\nu$	$\alpha$	$\Psi(1) = q$	$\Psi(1/2)$	$-\Psi'(1/2)_+$	$E_g$
0.002	1	$7.2 \times 10^{-5}$	15.748	3937	-81.4526
0.01	0.25	0.0127	1.0608	13.2601	-0.02710
0.01	1	0.031074	6.92821	346.41	-14.9334
0.01	10	0.037283	70.6965	35348.3	-16646.9
0.05	1	0.34647	2.83402	28.3402	-1.95903
0.05	10	0.511176	31.5911	3159.11	-3314
0.1	1	0.497576	1.78192	8.90962	-0.59964

**Table 2:** Parameters of the first excited state for  $\delta$ -function wells, for various choices of  $\nu$  and  $\alpha$ .  $E_1$  is the energy in  $[-1/2, 1/2]$ . For the other intervals, the energy is the  $E_g$  given in Table 1.

$\nu$	$\alpha$	$q$	$\epsilon$	$\Psi(1/2)$	$\Psi'(1/2)_-$	$E_1$
0.002	1	$7.2 \times 10^{-5}$	$1.5.2 \times 10^{-9}$	15.748	3937	-81.4526
0.01	0.25	0.0127	0.999838	1.0608	13.2613	-0.027094
0.01	1	0.031074	0.99903	6.9282	346.41	-14.9333
0.01	10	0.037283	0.998598	70.696	35348.3	-16646.9
0.05	1	0.34647	0.82356	2.8340	28.4417	-1.92445
0.05	10	0.511176	0.363395	31.591	3159.12	-3313.85
0.1	1	0.497576	0.424940	1.7819	9.28766	-0.526821

**Table 3:** Parameters of the highest state for  $\delta$ -function wells, for various choices of  $\nu$  and  $\alpha$ .  $E_h$  is the energy per interval.

$\nu$	$\alpha$	$\epsilon$	$\Psi(1/2)$	$\Psi'(1/2)_-$	$E_h$
0.002	1	$1.52 \times 10^{-9}$	15.748	3937	-81.4526
0.01	0.25	0.999838	1.0605	13.2565	-0.02707
0.01	1	0.99903	6.9282	346.41	-14.9332
0.01	10	0.998598	70.696	35348.3	-16646.9
0.05	1	0.82442	2.8213	28.213	-1.89582
0.05	10	0.363395	31.591	3159.11	-3313.84
0.1	1	0.516054	1.6527	8.26345	-0.40157
1	4.34	0.730536	0.2518	0.54642	-0.00038

## Figure Captions

**Figure 1:** (a) A typical wavefunction when the potential wells are very far apart ( $\nu \approx 0$ ).

(b) A typical wavefunction when the potential wells are closer together ( $\nu \ll 1$ ).

**Figure 2:** First excited state with the root at  $z = 0$ , for  $\delta$ -function wells.

**Figure 3:** The ground state, for  $\delta$ -function wells.

**Figure 4:** The potential  $u(z)$  for gaussian wells ( $g = 2.5$ ,  $b = 20$ ).

**Figure 5:** The ground state, the first excited state, and the highest state, for 20 gaussian wells with  $\nu = 0.01$ ,  $g=2.5$ ,  $b=20$ , with the corresponding energies per interval.

**Figure 6:** The ground state, the first excited state, and the highest state, for 20 gaussian wells with  $\nu = 0.05$ ,  $g=2.5$ ,  $b=20$ , with the corresponding energies per interval.

**Figure 7:** First excited state for gaussian wells with  $\nu = 0.1$ ,  $b = 20$ , and  $g=2.2$ ,  $2.5$  and  $5$ .

**Figure 8:** First excited state for gaussian wells with  $\nu = 0.1$ ,  $g = 2.5$  and  $b = 5$ ,  $10$ ,  $20$ , and  $25$ .